

Considerations on Neuberger's operator.

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We discuss new approaches to the numerical implementation of Neuberger's operator for lattice fermions and the possible use of block spin transformations.

Recently major progress has been made in the lattice discretization of fermionic fields. Starting from the overlap formulation, Neuberger has proposed a lattice Dirac operator which avoids the additive renormalization of fermion masses [1]. This operator satisfies an identity, the Ginsparg-Wilson relation [2], by which one can define exact lattice chiral symmetry [3]. Other lattice operators which satisfy the Ginsparg-Wilson relations have been obtained as implementations of the "perfect action" [4]. In this note we will concentrate on Neuberger's operator and we will follow his notation. If one defines the Wilson lattice operator as

$$(D_W \psi)(x) = \frac{\psi(x)}{\kappa} - \sum_{\mu} [(1 - \gamma_{\mu})U_{\mu}(x)\psi(x + \mu) + (1 + \gamma_{\mu})U_{\mu}(x - \mu)\psi(x - \mu)] \quad (1)$$

Neuberger's operator is

$$D = \frac{1}{2}(1 + V) \quad (2)$$

where the unitary operator V is given by

$$V = D_W(D_W^{\dagger}D_W)^{-1/2} \quad (3)$$

Provided the hopping parameter κ in Eq. 1 is chosen within a suitable range ($1/8 - 1/4$), Neuberger's operator defines a single flavor of massless lattice fermions, symmetric under chiral transformations.

Since in actual calculations the size of the matrix D_W is very large, for a practical implementation of Neuberger's operator it is crucial to find

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computationally efficient ways to calculate its action as well as the action of its inverse on any given vector. In some sense, the domain wall formulation of lattice fermions [5–7], which preceded the introduction of the operator of Eq. 2, provide a numerical procedure for its implementation. Other approximate methods have been proposed in [8–11]. Most of these numerical methods proceed through an approximation to the operator

$$e(H) \equiv H(H^2)^{-1/2} = \gamma_5 D_W (D_W^{\dagger} D_W)^{-1/2} \quad (4)$$

where $H \equiv \gamma_5 D_W$ is a Hermitian operator. Here we would like to focus directly on the operator V . We will make the assumption that $D_W^{\dagger} D_W$ has no zero eigenvalues, so that $(D_W^{\dagger} D_W)^{-1/2}$ is well defined (it can be argued that such zeroes are exceptional and irrelevant for the continuum limit).

Given any square matrix M such that $M^{\dagger} M$ has no zero eigenvalues, its "polar decomposition" is defined by

$$M = U A \quad (5)$$

where the matrix U is unitary and the matrix A is positive-definite Hermitian [12]. It mirrors the expression of a complex number in terms of its phase and modulus. The polar decomposition is unique, with $A = (M^{\dagger} M)^{1/2}$ and $U = M(M^{\dagger} M)^{-1/2}$. From Eq. 3 we see that the matrix V is the unitary factor in the polar decomposition of the Wilson lattice operator D_W . The main observation which we would like to make is that the unitary factor U in the polar decomposition of a matrix

M satisfies a maximum principle, namely U is the unique matrix which maximizes the expression $\text{Re Tr}(U'M^\dagger)$, where U' ranges over the entire space of unitary matrices of the same size as M :

$$\text{Re Tr}(UM^\dagger) = \text{Max}_{\{U' | U'^\dagger = I\}} \text{Re Tr}(U'M^\dagger) \quad (6)$$

The proof is straightforward. We write M in its polar form and write U' as $U' = UW$, where W is also unitary. This gives

$$\begin{aligned} \text{Re Tr}(U'M^\dagger) &= \text{Re Tr}[UW(M^\dagger M)^{1/2}U^\dagger] \\ &= \text{Re Tr}[W(M^\dagger M)^{1/2}] \end{aligned} \quad (7)$$

But $(M^\dagger M)^{1/2}$ is a positive-definite Hermitian matrix and we can therefore choose a basis where $(M^\dagger M)^{1/2} = \text{Diag}(\lambda_1, \lambda_2, \dots, \lambda_N)$, $\lambda_i > 0$. In this basis $\text{Re Tr}[W(M^\dagger M)^{1/2}] = \sum_i \text{Re}(w_{i,i})\lambda_i$ and since the eigenvalues λ_i are all positive and the unitarity of W implies $|w_{i,i}| \leq 1$, the maximum occurs for $W = I$, i.e. $U' = U$. Although this proof is very simple, the property expressed by Eq. 6 can hardly be found in books on matrix algebra [13]. Indeed very few pages, if any, are generally devoted to the polar decomposition itself.

Maximization and minimization principles have often proven very useful in numerical analysis, since they can form the starting point for efficient schemes of approximation. Here we would like to briefly mention a few possibilities. Assuming that one is interested in calculating either $D\chi$ or $D^{-1}\chi$, one could construct the Krylov space spanned by the vectors obtained acting with H on χ (this space also underlies the approximation methods of [8–11]):

$$\chi_k = H^k \chi \quad k = 0 \dots n \quad (8)$$

In order to respect the symmetry properties of V under γ_5 transformation, it is desirable to augment the basis by considering separately the two projections

$$\chi_{ks} = \frac{1 + s\gamma_5}{2} \chi_k \quad s = \pm 1 \quad (9)$$

For sufficiently large n this basis would become overcomplete, but we must work under the assumption that values of n much smaller than the

dimensionality N of the full vector space will produce reasonable approximations. We will finally denote by η_{ks} an orthonormalized basis in the space spanned by the vectors χ_{ks} . (This will require forming a number of scalar products of order n^2 . We are working under the hypothesis that the values of n one must consider make it feasible both to calculate these scalar products and to store the vectors η_{ks} .) At this point the maximization of $\text{Re Tr}(U'M^\dagger)$ may be restricted to unitary operators in the space E spanned by the vectors η_{ks} , namely

$$U' = \sum_{ks, k's'} v_{ks, k's'} \eta_{ks} \eta_{k's'}^\dagger + I_{\bar{E}} \quad (10)$$

where $I_{\bar{E}}$ denotes the identity in the complement of E . Maximizing $\text{Re Tr}(U'M^\dagger)$ one finds that the $(2n) \times (2n)$ matrix $v_{ks, k's'}$ is the unitary factor in the polar decomposition of the truncated matrix $\eta_{k's'}^\dagger D_W \eta_{ks}$. As already mentioned above, this procedure will work only if reasonably small values of n can produce satisfactory approximations.

The truncation of Eq. 10 does not represent, however, the only way to take advantage of the maximization principle. Another possibility is to assume an approximately ultralocal form for V . V is known to be local [10] and the approximation would consist in making it ultralocal. Imposing such a condition on a unitary operator may be problematic, but one could write $V = \exp(iK)$ with $K^\dagger = K$ and truncate to 0 the matrix elements of K which exceed a maximum separation. Otherwise, one could try to construct a better approximation to V by the refinement of a first approximation: $V = V' V^{(0)}$. A particularly appealing possibility is to take for $V^{(0)}$ the operator defined by a coarsening of the lattice obtained by a blocking similar to those used in multigrid algorithms. Multigrid techniques have been tried for lattice fermions, but their application to the Wilson lattice operator [14] turned out to be only marginally effective, most likely because of the presence of an additive mass renormalization. Neuberger's operator is not affected by a similar renormalization and this offers the hope that multigrid methods may work much better. In a multigrid approximation, one divides the

lattice in cells of 2^d sites (for one level of coarsening). The gauge must be fixed within the cells, in order to make the transport factors as close as possible to the identity. Since this gauge fixing is local to the cells, it is not computationally expensive. The local gauge fixing leaves the freedom of performing gauge transformations common to all the sites within the cells. This becomes a gauge symmetry of the blocked lattice. After the local gauge fixing it makes sense to define a projection over the average cell fermionic fields. We define new basis vectors

$$\eta_X^{(0)} = 2^{-d/2} \sum_y \eta_{2X+y} \quad (11)$$

where the vectors η_x form a local basis for the fermions (spin and color indices are left implicit), x and X denote the integer valued coordinates of the original and coarse lattices, respectively, and y are d -dimensional vectors with components that take value 0 or 1. We can now define

$$V^{(0)} = \sum_{XX'} v_{XX'}^{(0)} \eta_X^{(0)} \eta_{X'}^{(0)\dagger} + I_{\bar{E}^{(0)}} \quad (12)$$

where $I_{\bar{E}^{(0)}}$ denotes the identity in the complement of the space spanned by $\eta_X^{(0)}$. The matrix elements $v_{XX'}^{(0)}$ can then be determined by maximizing $\text{ReTr}(V^{(0)} D_W^\dagger)$. Alternatively, one could maximize $\text{ReTr}(V^{(0)} D_W^{(0)\dagger})$, where $D_W^{(0)}$ denotes a coarse lattice Wilson, obtained by defining transport factors $U_X^{(0)\mu}$ between neighboring cells as the $SU(3)$ matrices that maximize $\text{ReTr}(U_X^{(0)\mu} S_X^{\mu\dagger})$, where S_X^μ denotes the sum of the transport factors U_x^μ connecting the boundary sites of the cells in the original lattice. In both cases, the size of the matrix to determine is reduced by $2^d \times 2^d$.

Of course the crucial question is whether these or similar computational procedures can provide a sufficiently accurate approximation to Neuberger's operator without excessive usage of CP time and memory. We are currently working to test the approximations outlined above and hope to report on our results in the near future. At the same time, we hope that this communication may open new avenues in the quest for efficient algorithms for lattice fermions.

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